Ethyl heptanoate
106-30-9 | DTXSID1040112

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 11.4

Global applicability domain: Inside

Local applicability domain index: 5.52e-01

Confidence level: 5.51e-01

Nearest Neighbors from the Training Set

Image not found
Butyl ether
Measured: 72.4
Predicted: 32.3

Image not found
Molinate
Measured: 25.7
Predicted: 14.8

Image not found
Acetamide, N-methyl-N-phenyl-
Measured: 1.51
Predicted: 2.53

Image not found
Carbaryl
Measured: 8.91
Predicted: 5.04